

Spontaneous spin switching via substrate-induced decoherence

Jean-Pierre Gauyacq

*Institut des Sciences Moléculaires d'Orsay, ISMO, Unité mixte CNRS-Univ Paris-Sud,
UMR 8214, Bâtiment 351, Univ Paris-Sud, 91405 Orsay CEDEX, France*

Nicolás Lorente

*ICN2 - Institut Catala de Nanociencia i Nanotecnologia,
Campus UAB, 08193 Bellaterra (Barcelona), Spain
CSIC - Consejo Superior de Investigaciones Científicas,
ICN2 Building, 08193 Bellaterra (Barcelona), Spain*

(Dated: July 4, 2014)

We analyze the spontaneous switching between the two Néel states of Fe chains on $\text{Cu}_2\text{N}/\text{Cu}(100)$, experimentally studied by Loth et al. [Science **335**, 196 (2012)]. We show that, in the experimental low-temperature regime ($T \approx 1$ K), decoherence induced by substrate electrons deeply modifies the dynamics of the chain magnetization. The Rabi oscillations associated to quantum tunneling of the isolated chain are replaced by an irreversible decay of considerably longer characteristic time. The computed switching rate is small, rapidly decreasing with chain length, with a $1/T$ behavior and in good agreement with the experiment. Quantum tunneling is only recovered as the switching mechanism at extremely low temperatures, the corresponding cross-over moving rapidly to further low temperatures as the chain length is increased.

PACS numbers: 75.10.Pq, 75.10.Jm, 75.50.Ee, 68.37.Ef

Decoherence is becoming a central concept in the study of quantum objects [1–3]. It is caused by the influence of the environment on the studied object that leads to the suppression of interference between quantum states and hence to a classical behavior of the object. The presence of decoherence is ubiquitous: from atomic optics [4–6], to the foundations of quantum mechanics and the passage to the classical world [1–3], including the environment-imposed limitations in quantum information and computations [7, 8]. Decoherence also plays an important role in surface science [9], like in the scattering and localization of atoms on surfaces, in the dynamics of surface-confined electronic states [10, 11] or in surface-adsorbed spins [9, 12]. For an adsorbate, the substrate acts as a bath of electronic, phononic and nuclear excitations that cannot be neglected in the study of adsorption. The scanning tunneling microscope (STM) has permitted us to have unprecedented insight on adsorbed quantum objects. Indeed, the STM has been used to unveil the static and dynamical properties of spins on surfaces [13–16]. In this context, decoherence plays a particular important role [12, 17, 18].

Recently, Loth and collaborators [19] measured the dynamical properties of antiferromagnetically coupled atomic Fe chains on $\text{Cu}_2\text{N}/\text{Cu}(100)$. They observed a Néel spin ordering in chains with an even number of atoms, i.e. all the spins are aligned on the same direction with alternate directions along the chain. Their experiment revealed that the chains could switch from one Néel state to the opposite Néel state via either electron injection from an STM tip or by increasing the sample temperature. The tunneling electron-induced regime showed a clear threshold when the electron energy was

large enough to excite an intermediate magnetic excited state of the chain that greatly enhanced the switching [19, 20]. When studying the temperature-induced flipping of the local moments of the chains, [19] two different regimes were found: (i) a high-temperature regime where the switching rate followed an Arrhenius exponential behavior with a finite activation energy that is in good agreement with the energy of the intermediate state of the tunneling electron-induced process and (ii) a low-temperature regime, flat as a function of inverse of temperature, reminiscent of the customary quantum tunneling regimes of atom diffusion [21, 22] or of magnetic processes [23–26]. Regime (i) is analogous to the STM electron-driven process and it has been carefully analyzed in the literature [19, 20], however, regime (ii) has received less attention due to the conceptual difficulties that it presents. Indeed, we show here that the very low-switching rate of regime (ii) and its weak temperature dependence are not due to a tunneling process [19], but are rather an effect of the fast substrate-induced decoherence; this places decoherence at the heart of spin stability in a few-atom devices.

Using the theory developed in Refs. [27, 28], we have evaluated the switching rate between the above Néel states. Only when decoherence is included, can the experimental data be explained. Let us suppose that initially, the Fe chain is prepared in one of the two Néel states. In the absence of decoherence, a Rabi oscillation sets in between the two Néel states, because the Néel states are broken-symmetry solutions of the chain's Hamiltonian [20]. The period of the Rabi oscillation is proportional to the inverse of the energy separation between the two lowest-lying eigenstates of the chain, fol-

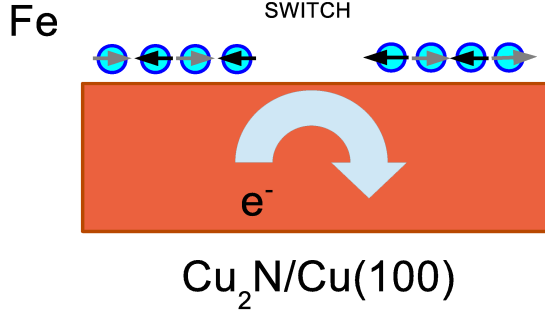


FIG. 1: Switch between the two Néel states of an Fe atomic chain on a $\text{Cu}_2\text{N}/\text{Cu}(100)$ substrate. The thermal electrons from the substrate cause the decoherence of the chain's spin state. The joint action of the high-order indirect Heisenberg coupling between the Néel states and of the substrate-induced decoherence results in the spontaneous switching of the chain between the two magnetization states.

lowing the customary quantum-tunneling picture [25, 26]. These oscillations are many orders of magnitude faster than the measured switching rates [19]. However, when decoherence induced by thermal electron-hole pair excitations of the substrate is considered, Fig. 1, the oscillations are damped and the decoherence produces the collapse of the spin state into one of the two Néel states with equal probability.

The Fe chain is described by a set of local spins, \vec{S}_i , in an anisotropic environment and coupled by a first-neighbor Heisenberg exchange, J , [19, 20, 29–32]:

$$\hat{H} = \sum_{i=1}^{N-1} (J\vec{S}_i \cdot \vec{S}_{i+1} + g\mu_B \vec{S}_i \cdot \vec{B}) + DS_{i,z}^2 + E(S_{i,x}^2 - S_{i,y}^2). \quad (1)$$

The local Fe spins are $S_i = 2$, where i is the atom index for N Fe atoms. Local axial, D , and transverse, E , magnetic anisotropies have been included together with the Zeeman term due to an external field \vec{B} . The actual values of J , D , E and g are taken from the study on adsorbed dimers by Bryant *et al* [33]. Due to the above interactions and the integer total spin, the ground state, $|GS\rangle$, is not degenerate. In systems like the present one with a large D anisotropy term, the system is close to an Ising model. The first excited state, $|EXC\rangle$, has a very small excitation energy that we express as $2V$. Both $|GS\rangle$ and $|EXC\rangle$ correspond to the superposition of many configurations of local spins, with large weights of equal value on the two Néel states. From these, one can then define the Néel states, $|N_1\rangle$ and $|N_2\rangle$, as linear combinations of the two low lying states:

$$\begin{aligned} |N_1\rangle &= \frac{1}{\sqrt{2}}(|GS\rangle + |EXC\rangle), \\ |N_2\rangle &= \frac{1}{\sqrt{2}}(|GS\rangle - |EXC\rangle). \end{aligned} \quad (2)$$

With this definition, the two Néel states are not pure Néel configurations of local spins, but include correlation effects that are important in anti-ferromagnetic chains [20, 32, 34]. The above excitation energy, $2V$, then appears as twice the coupling between the two Néel states, Eq. (2). The coupling V is very weak and it is due to the correlated nature of the Néel states. Actually, it is possible to go from $|N_1\rangle$ to $|N_2\rangle$ by applying several times the Heisenberg exchange or the anisotropy E operators in Eq. (1). The two states are then weakly coupled via a high-order indirect interaction involving many intermediate spin configurations. Due to this high-order character, the coupling V is very sensitive to the choice of parametrization in Eq. (1).

When the chain is prepared in the Néel state $|N_1\rangle$, the chain evolves under the above effective coupling, V , leading to Rabi oscillations between the two states $|N_1\rangle$ and $|N_2\rangle$ with period $T_{\text{Rabi}} = \pi\hbar/V$. This corresponds to a quantum tunneling phenomenon and would account for the periodic spontaneous switching of magnetization of the chain if it were isolated.

The effect of the substrate can be included using the density matrix of the system, $\hat{\rho}_T = |\Psi\rangle\langle\Psi|$ where $|\Psi\rangle$ is the state of the full system. By tracing out the environment's degrees of freedom, we are left with the reduced density matrix for the spin degrees of freedom of the chain [35]:

$$\hat{\rho} = \sum_j \langle j|_{\text{env}} (|\Psi\rangle\langle\Psi|) |j\rangle_{\text{env}}, \quad (3)$$

where $|j\rangle_{\text{env}}$ is a complete basis set of the environment system, *env*. The time evolution of the reduced density matrix is then given by:

$$i\hbar \frac{d\hat{\rho}}{dt} = [\hat{H}_{\text{red}}, \hat{\rho}] + \hat{R}(\hat{\rho}), \quad (4)$$

where \hat{H}_{red} is the 2×2 Hamiltonian matrix for the space spanned by the two Néel states (the two diagonal energies are equal and the two non-diagonal terms are equal to the effective coupling, V). \hat{R} takes into account the effect of the environment in the reduced density matrix evolution, it is given by the expresion [35, 36]:

$$\hat{R}(\hat{\rho}) = -i\Gamma (|N_1\rangle\rho_{12}\langle N_2| + |N_2\rangle\rho_{21}\langle N_1|), \quad (5)$$

where ρ_{12} and ρ_{21} are the non-diagonal density matrix elements between the two Néel states, $|N_1\rangle$ and $|N_2\rangle$. The quantity Γ/\hbar is the decoherence rate of a Néel state, given by the inverse of the pure dephasing time, T_2^* . The substrate is not magnetic and hence the decoherence rate is the same for the two Néel states. Note that Eq.(4) has been written in the Néel-state basis, implicitly assuming the decoherence term to be much larger than the effective coupling, V .

The resulting set of equations can be easily solved by defining the population difference: $\Delta P = \rho_{11} - \rho_{22}$. The

solution is

$$\Delta P = \frac{-4V^2}{\sqrt{\Gamma^2 - 16V^2}} \left(\frac{e^{\omega_+ t}}{\omega_+} - \frac{e^{\omega_- t}}{\omega_-} \right), \quad (6)$$

when initially the chain is in the $|N_1\rangle$ state. The values of ω_{\pm} are $0.5(-\Gamma \pm \sqrt{\Gamma^2 - 16V^2})$. Then, for long times, Eq. (6) leads to equal populations of the two Néel states, $\rho_{11} = \rho_{22}$. In parallel, non-diagonal terms (coherences) die out on the same time scale, so that the final state of the evolution is an equal and incoherent population of the two Néel states.

In the present case, the decoherence rate is very fast compared to the Rabi evolution, $\Gamma \gg V$ (or equivalently $T_{Rabi} \gg T_2^*$). Therefore, the population difference can be approximated by:

$$\Delta P \approx e^{-\frac{4V^2 t}{\hbar\Gamma}}, \quad (7)$$

from which we obtain the *switching rate* between Néel states $|N_1\rangle$ and $|N_2\rangle$:

$$\frac{1}{\tau_{1 \rightarrow 2}} = \frac{2V^2}{\hbar\Gamma} = \frac{1}{T_{Rabi}} \frac{2\pi V}{\Gamma} \quad (8)$$

The decoherence rate, Γ/\hbar , accounts for the loss of coherence of the evolving spin state due to collisions with hot electrons from the substrate. Its calculation is akin to the calculation of de-excitation of spin states on surfaces [28, 37] except that the spin state does not change. Each collision entails a change in the state phase and hence the decoherence of the evolving spin state, $|N_1\rangle$ or $|N_2\rangle$. The decoherence rate can be expressed as the addition of electron collisions with each atom of the chain. As shown in Ref. [37], the electron collision rate can be separated in three parts, and the total rate can be expressed as

$$\Gamma = NT_{Fe}(E_F) \frac{k_B T}{2\pi} P_{Spin}(N_1 \rightarrow N_1). \quad (9)$$

The first factor is the electron transmission at the Fermi energy, $NT_{Fe}(E_F)$, that takes into account the electron flux through the N Fe atoms of the chain, where $T_{Fe}(E_F)$ typically amounts to 1 [37] [40]. The second factor accounts for the number of electrons that can collide with the target. These hot electrons are given by the convolution of the electron and hole Fermi functions [38]. At low temperature, T , the second term is just $\frac{k_B T}{2\pi}$. Finally, $P_{Spin}(N_1 \rightarrow N_1)$ represents the elastic scattering probability for an electron scattered by an atom in the chain; it is not a trivial number since it depends on all the possible spin transitions of the target. It amounts typically to 0.8-0.9 for the various chains (see a discussion in [20]).

For a six-atom Fe chain on $\text{Cu}_2\text{N}/\text{Cu}(100)$, the decoherence rate is indeed very fast. The effective coupling, V , is 1.85×10^{-6} meV, while the decoherence rate is 0.14 meV at $T = 2$ K. Thus, the decoherence rate is much

larger than the Rabi frequency between the Néel states, justifying the above approach. The consequence of fast decoherence is clearly seen in Fig. 2. In (a), the evolution of the population of state $|N_1\rangle$ in the presence of decoherence is shown as a function of time, for an initial population of $|N_1\rangle$ equal to 1. It decreases exponentially to 0.5, and the system becomes an incoherent superposition of states 1 and 2. Figure 2 (a) also illustrates the effect of a measurement as performed e.g. in an STM experiment: at an arbitrarily chosen time ($t = 0.02$ s), a measurement is performed that, for example, finds the system in state $|N_1\rangle$; this leads to a restart of the population evolution that again relaxes towards an incoherent situation.

In Fig. 2 (b) the Rabi evolution is shown for comparison. The time evolution is orders of magnitude slower in the presence of decoherence (see e.g. Eq. (8)). The quantal state of the chain loses its phase many times before a Rabi oscillation could be performed (before quantum tunnelling could set in) and the decoherence strongly hampers the switching rate between the two spin states. The difference between cases (a) and (b) goes beyond the difference in time scales. Rabi oscillations (b) correspond to a reversible coherent evolution between the two Néel states. Decoherence results in an irreversible evolution toward an incoherent superposition of the two Néel states and thus explains the experimental observation by Loth *et al.* [19] of Néel states and not of the ground state of the isolated system. However, decoherence is not the only physical effect at play, the relative values of magnetic anisotropy (D and E) and exchange couplings (J) are very important. Indeed, Néel states have not been observed for chains with an even number of Mn atoms [29] due to the negligible longitudinal anisotropy, D in Eq. (1).

The switching rate between the two Néel states, $1/\tau_{1 \rightarrow 2}$, obtained in our calculations (Eq. (8)), is displayed in Figure 3. It shows the different rates as functions of the number of atoms in the chain. The switching rate presents a fast exponential decrease with the number of atoms in quantitative agreement with the switching rates measured for Fe_6 and Fe_8 [19]. The exponential decrease with increasing length is due to the exponential behavior of the Rabi frequency, also shown in Fig. 3. Indeed, when increasing the chain length, the indirect coupling between Néel states becomes of higher and higher order in J , Eq. (1), leading to the exponential decrease of the effective coupling, V , with the number of atoms, N . However, the decoherence rate slightly increases with chain length, due to the increase of the number of atoms, N , that can be hit by substrate electrons, Eq. (9).

Our calculations show that the switching rate presents *three* regimes as a function of temperature. (i) A high-temperature regime where hot substrate electrons have enough energy to excite higher-lying excited states in the chain, triggering an efficient indirect switching process,

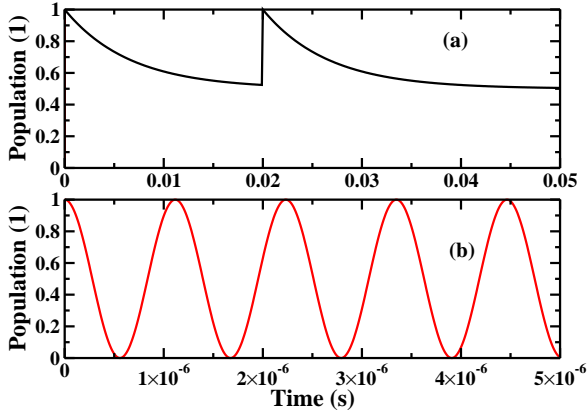


FIG. 2: (a) Time evolution of the Néel-state population in the presence of decoherence. A Fe_6 chain is initially prepared in the $|N_1\rangle$ state, and decoherence leads to an exponential decline of its population. At ~ 0.02 s, the chain is either in the $|N_1\rangle$ or the $|N_2\rangle$ states with equal probability. We assume that a measurement is performed at ~ 0.02 s in order to determine the chain's state, and hence the population is determined and the evolution starts again. (b) For comparison, the $|N_1\rangle$ -state population is shown in the absence of decoherence. The evolution is of the Rabi type and the oscillation is orders of magnitude faster than when decoherence is taken into account as in (a) (note the change in time scale).

such as the one described in Refs. [19, 20]. (ii) A second regime of intermediate temperatures where indirect transitions are not possible due to energy conservation. This second regime, studied in detail in the present work, is dominated by hot-electron decoherence and presents a $\sim 1/T$ behavior. In front of the exponential behavior of the high- T regime, this $1/T$ is slowly varying and can be easily confused with a tunneling behavior. (iii) Finally, at extremely low temperatures, decoherence becomes negligible and Rabi oscillations dominate. In this very-low-temperature regime, the chain's evolution can be described via Hamiltonian (1), and truly corresponds to a quantum tunneling regime. In this regime, a decay term for the excited state, $|EXC\rangle$, population has to be included. For the six-atom chain, the decoherence rate becomes equal to the Rabi frequency in the μK range and as the chain length increases, the cross-over from decoherence-dominated to quantum tunneling behavior is rejected to further lower temperatures.

As the chain length shortens, the importance of decoherence in the spin dynamics reduces. The situation of Fe dimers is different from that of longer chains. At 2 K, (see Fig. 3), all rates are roughly of the same order of magnitude, so that the system is not decoherence-dominated. This is the case of Fe dimers at 330 mK [33], where the decoherence rate is smaller than the coupling V and consistently, the conductance spectrum shows a low-energy

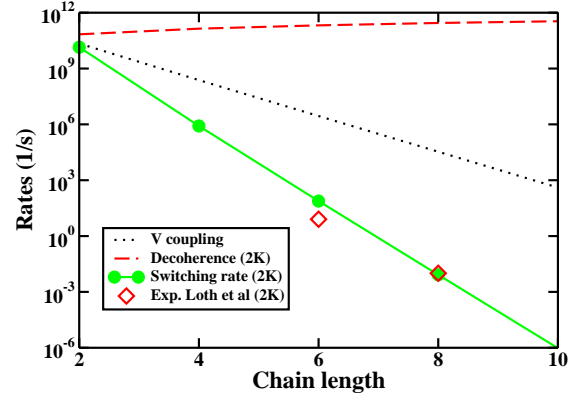


FIG. 3: Rates for the various processes in the Fe chains as a function of the number of atoms for a substrate temperature equal to 2K. The available experimental data (red diamonds) for the switching rate are also shown [19]. The full green line is the present computed switching rate between the two Néel states. The V coupling and the decoherence rate are plotted as dotted and dashed lines, respectively.

threshold due to the excitation of the $|EXC\rangle$ state.

In summary, we have evaluated the spontaneous switching rate between the two possible Néel states of atomic Fe chains adsorbed on $\text{Cu}_2\text{N}/\text{Cu}(100)$ [19]. We show that the quantum tunneling associated with Rabi oscillations in this system is deeply modified by the presence of a strong substrate-induced decoherence process, leading to a considerable slowing down of the switching process and to a change of its character. The decoherence-assisted process leads to the relaxation of the chain magnetic state toward an incoherent population of both Néel states, instead of the Rabi oscillations of the quantum tunneling process. At high temperature, indirect transitions [20] induced by hot substrate electrons lead to an Arrhenius-type of T -dependence [19]. In the few-Kelvin range, the decoherence-assisted switching mechanism takes over, in quantitative agreement with the experiment, and with the correct scaling with chain length, the switching rate slowing down exponentially with the chain length. Only at extremely low temperatures (below the μK range for the six-atom chain and exponentially lower for longer chains) does quantum tunneling prevail over the above decoherence-assisted mechanism.

Decoherence appears as a key phenomenon in the switching of magnetization at surfaces, and it is quite remarkable that decoherence is able to dominate the spin dynamics down to unattainable temperatures even for a spin system of only a few atoms.

N.L. acknowledges financial support from Spanish MINECO (Grant No. MAT2012-38318-C03-02 with joint financing by FEDER Funds from the European Union)

and fruitful discussions with J. Fernández-Rossier.

-
- [1] W. H. Zurek, Phys. Lett. A **44**, 36 (1991).
- [2] W. H. Zurek, Rev. Mod. Phys. **75**, 715 (2003), URL <http://link.aps.org/doi/10.1103/RevModPhys.75.715>.
- [3] M. Schlosshauer, Rev. Mod. Phys. **76**, 1267 (2005), URL <http://link.aps.org/doi/10.1103/RevModPhys.76.1267>.
- [4] S. Haroche, Rev. Mod. Phys. **85**, 1083 (2013), URL <http://link.aps.org/doi/10.1103/RevModPhys.85.1083>.
- [5] P. Jacquod and C. Petitjean, Advances in Physics **58**, 67 (2009).
- [6] B.-S. K. Skagerstam, U. Hohenester, A. Eiguren, and P. K. Rekdal, Phys. Rev. Lett. **97**, 070401 (2006), URL <http://link.aps.org/doi/10.1103/PhysRevLett.97.070401>.
- [7] D. DiVincenzo, Fortschritte der Physik **48**, 771 (2000).
- [8] F. Luis, O. Roubeau, and G. Aromi, Proceedings of the 2nd AtMol European Workshop (2012).
- [9] G. Doyen and D. Drakova, Surface Science **603**, 1579 (2009).
- [10] U. Höfer, I. L. Shumay, C. Reuß, U. Thomann, W. Wal-lauer, and T. Fauster, Science **277**, 1480 (1997).
- [11] F. E. Olsson, A. G. Borisov, M. Persson, N. Lorente, A. K. Kazansky, and J. P. Gauyacq, Phys. Rev. B **70**, 205417 (2004), URL <http://link.aps.org/doi/10.1103/PhysRevB.70.205417>.
- [12] F. Delgado and J. Fernández-Rossier, Phys. Rev. Lett. **108**, 196602 (2012), URL <http://link.aps.org/doi/10.1103/PhysRevLett.108.196602>.
- [13] A. J. Heinrich, J. A. Gupta, C. P. Lutz, and D. M. Eigler, Science **306**, 466 (2004).
- [14] C. F. Hirjibehedin, C.-Y. Lin, A. F. Otte, M. Termes, C. P. Lutz, B. A. Jones, and A. J. Heinrich, Science **317**, 1199 (2007).
- [15] S. Loth, M. Etzkorn, C. P. Lutz, D. M. Eigler, and A. J. Heinrich, Science **329**, 1628 (2010).
- [16] A. A. Khajetoorians, B. Chilian, J. Wiebe, S. Schwalow, F. Lechermann, and R. Wiesendanger, Nature **467**, 1084 (2010).
- [17] F. Delgado, C. Hirjibehedin, and J. Fernández-Rossier, arXiv:1401.7272 [cond-mat.mes-hall] -, (2014).
- [18] F. Delgado, S. Loth, M. Zielinski, and J. Fernández-Rossier, arXiv:1405.3304 [cond-mat.str-el] -, (2014).
- [19] S. Loth, S. Baumann, C. P. Lutz, D. M. Eigler, and A. J. Heinrich, Science **335**, 196 (2012).
- [20] J.-P. Gauyacq, S. M. Yaro, X. Cartoixa, and N. Lorente, Phys. Rev. Lett. **110**, 087201 (2013), URL <http://link.aps.org/doi/10.1103/PhysRevLett.110.087201>.
- [21] T. R. Mattsson, U. Engberg, and G. Wahnström, Phys. Rev. Lett. **71**, 2615 (1993), URL <http://link.aps.org/doi/10.1103/PhysRevLett.71.2615>.
- [22] L. J. Lauhon and W. Ho, Phys. Rev. Lett. **85**, 4566 (2000), URL <http://link.aps.org/doi/10.1103/PhysRevLett.85.4566>.
- [23] B. Barbara and E. M. Chudnovsky, Phys. Lett. A **145**, 205 (1990).
- [24] N. V. Prokof'ev and P. C. E. Stamp, Journal of Physics: Condensed Matter **5**, L663 (1993), URL <http://stacks.iop.org/0953-8984/5/i=50/a=002>.
- [25] D. Gatteschi and R. Sessoli, Angewandte Chemie International Edition **42**, 243 (2003), ISSN 1521-3773, URL <http://dx.doi.org/10.1002/anie.200390091>.
- [26] S. Hill, Polyhedron **64**, 128 (2013), symposia-in-Print (by invitation).
- [27] N. Lorente and J.-P. Gauyacq, Phys. Rev. Lett. **103**, 176601 (2009), URL <http://link.aps.org/doi/10.1103/PhysRevLett.103.176601>.
- [28] J.-P. Gauyacq, N. Lorente, and F. Dutilh Novaes, Progress in Surface Science **87**, 63 (2012).
- [29] C. F. Hirjibehedin, C. P. Lutz, and A. J. Heinrich, Science **312**, 1021 (2006).
- [30] J. Fransson, Nano Letters **9**, 2414 (2009), pMID: 19507889.
- [31] J. Fernández-Rossier, Phys. Rev. Lett. **102**, 256802 (2009), URL <http://link.aps.org/doi/10.1103/PhysRevLett.102.256802>.
- [32] J. P. Gauyacq and N. Lorente, Phys. Rev. B **83**, 035418 (2011), URL <http://link.aps.org/doi/10.1103/PhysRevB.83.035418>.
- [33] B. Bryant, A. Spinelli, J. J. T. Wagenaar, M. Gerrits, and A. F. Otte, Phys. Rev. Lett. **111**, 127203 (2013), URL <http://link.aps.org/doi/10.1103/PhysRevLett.111.127203>.
- [34] J. des Cloizeaux and J.J.Pearsson, Phys. Rev. **128**, 2131 (1962).
- [35] C. Cohen-Tannoudji, J. Dupont-Roc, and G. Grynberg, Processus d'interaction entre photons et atomes (EDP Sciences/CNRS Editions, Les Ulis, 2001).
- [36] K. Mölmer, Y. Castin, and J. Dalibard, J. Opt. Soc. Am. B **10**, 524 (1993).
- [37] F. D. Novaes, N. Lorente, and J.-P. Gauyacq, Phys. Rev. B **82**, 155401 (2010), URL <http://link.aps.org/doi/10.1103/PhysRevB.82.155401>.
- [38] J. Lambe and R. C. Jaklevic, Phys. Rev. **165**, 821 (1968), URL <http://link.aps.org/doi/10.1103/PhysRev.165.821>.
- [39] F. D. Novaes, N. Lorente, and J.-P. Gauyacq, Work in progress (2014).
- [40] Recent calculations by [39] on individual Fe adatoms on Cu₂N/Cu(100) yielded $T_{Fe}(E_F)$ values in the same range as those obtained for Mn adsorbates in [37].